Attention is all you need: utilizing attention in AI-enabled drug discovery

Year: 2023 | Citations: 246 | Authors: Yang Zhang, Caiqi Liu, Mujiexin Liu, Tianyuan Liu, Hao Lin

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Abstract

Abstract Recently, attention mechanism and derived models have gained significant traction in drug development due to their outstanding performance and interpretability in handling complex data structures. This review offers an in-depth exploration of the principles underlying attention-based models and their advantages in drug discovery. We further elaborate on their applications in various aspects of drug development, from molecular screening and target binding to property prediction and molecule generation. Finally, we discuss the current challenges faced in the application of attention mechanisms and Artificial Intelligence technologies, including data quality, model interpretability and computational resource constraints, along with future directions for research. Given the accelerating pace of technological advancement, we believe that attention-based models will have an increasingly prominent role in future drug discovery. We anticipate that these models will usher in revolutionary breakthroughs in the pharmaceutical domain, significantly accelerating the pace of drug development.